Spreading of Liquid Monolayers on Chemically Patterned Substrates -- Kinetic Monte Carlo Simulations and the Continuum Limit

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Manipulating fluids at the nanoscale within networks of channels or chemical lanes is a crucial challenge in developing small-scale devices to be used in microreactors or chemical sensors. Ultra-thin (i.e., monolayer) films observed in the spreading of nano-droplets or upon extraction from reservoirs in capillary rise geometries, represent an extreme limit that is of physical and technological interest since the dynamics is governed solely by capillary forces.

We have studied the transport of liquid monolayers extracted from reservoirs in contact with a chemically heterogeneous flat surface. The surfaces studied had domains of different wettability patterned using a simple lattice gas with interacting particles model for the fluid and assuming that the difference in wettability may be modeled solely by different chemical potentials.

Using kinetic Monte Carlo simulations of this model, we have studied the case of very simple patterns consisting of stripes with different wettability oriented along or perpendicular to the direction of flow, and the behavior at a T-junction. Our simulations indicate that it is possible to achieve lateral confinement of the flow at relatively low chemical potential differences. Surprisingly, in the case of the confined flow along a wettable stripe the mass transport is faster along the edges of the stripe than through the middle region. The simulations also indicate that in this case the advancing edge of the liquid follows a square-root dependence on time at very long times, with a prefactor dependent on the width of the stripe. This regime is preceded by very long transients. In contrast, for non-wettable stripes oriented transversal to the direction of flow our simulations suggests that flooding of this region occurs, followed by rupture of the film. This occurs even for very large differences in chemical potential between the wettable and the non-wettable regions. The prefactor in the square root time dependence mentioned above and its dependence on the stripe width, in the asymptotic regime (long times and large spatial scales), is analyzed using numerical solutions of a non-linear, uphill diffusion equation derived from the microscopic dynamics in the continuum limit.